Healthcare Predictive Modeling with Graph Networks

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https://github.com/acomphealth/odsc2022-mimic-graphnet

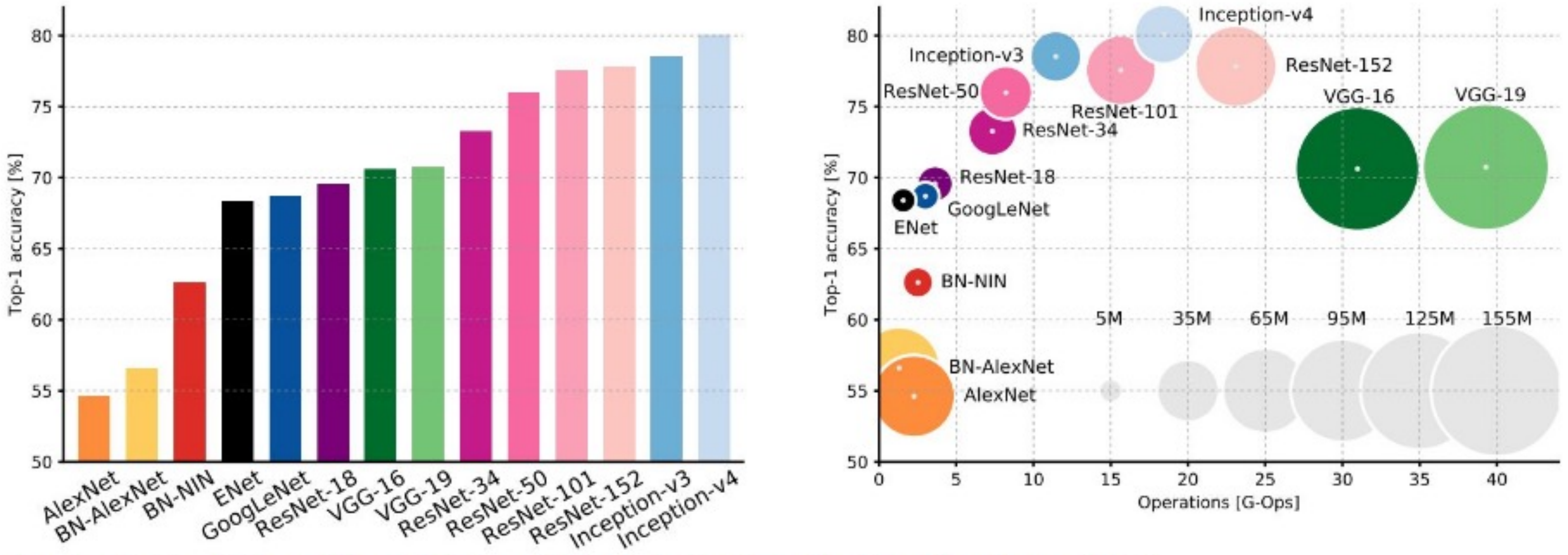
Overview

- Why graph networks?
- Limitations of traditional tools when applied to graphs
- Graph models in healthcare and biotech
- Impact of data models on predictive models
- Tools to enable AI with graph models

Computational Healthcare

The interdisciplinary application of innovative data science tools to address health-related questions and problems

Advancements in AI/ML



An Analysis of Deep Neural Network Models for Practical Applications, 2017.

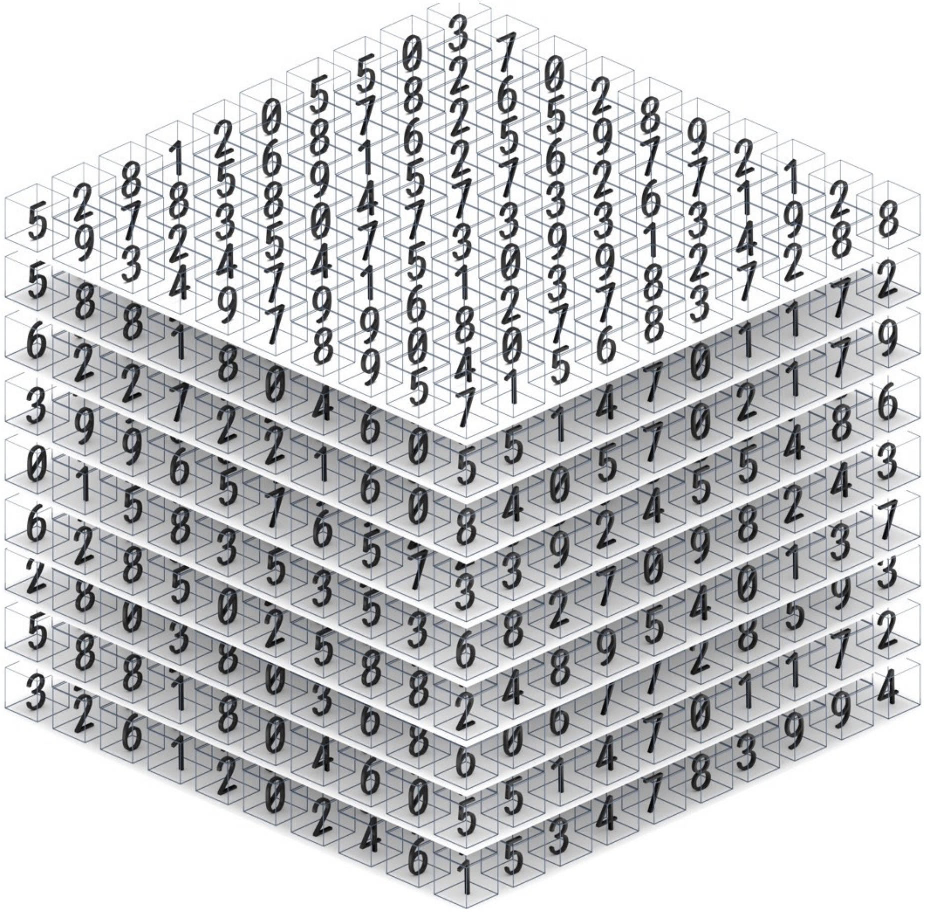
Features + Relationships

0	0	152	244	255	255
0	152	244	255	255	0
0	0	0	152	244	0

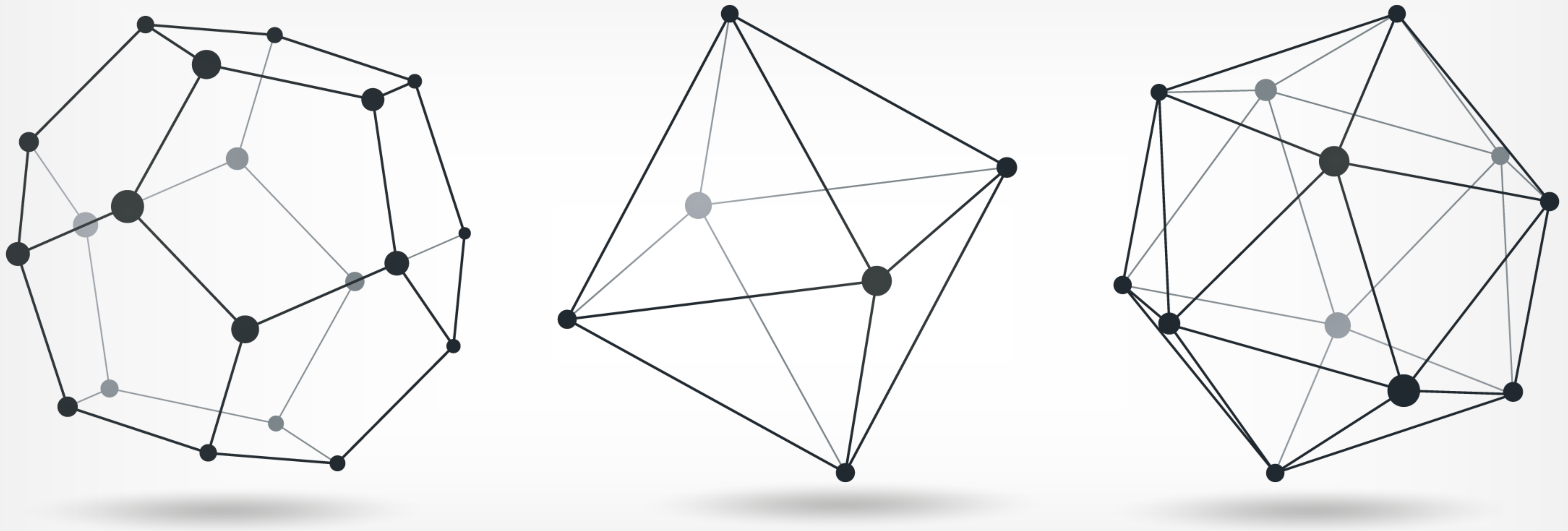
Features + Relationships

0	0	152	244	255	255
0	152	244	255	255	0
0	0	0	152	244	0

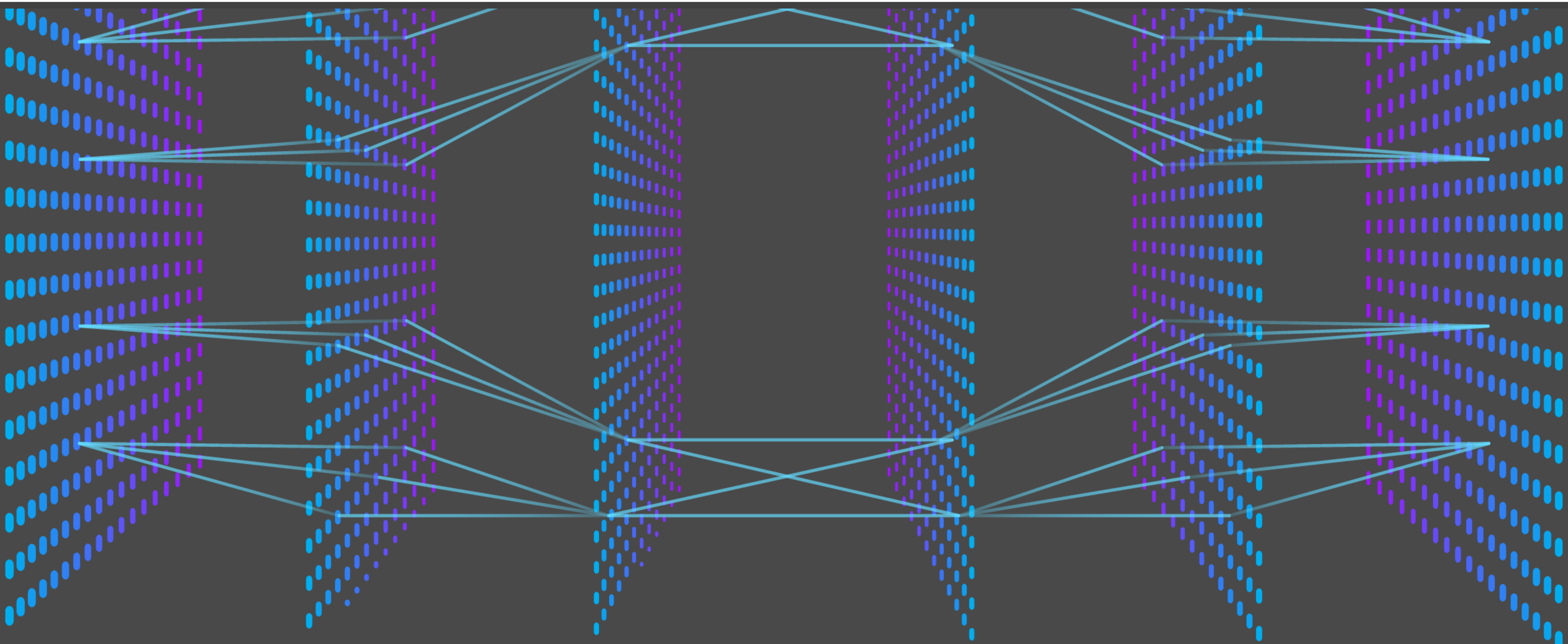
Limited Dimensions



Graphs: *The Next Frontier*

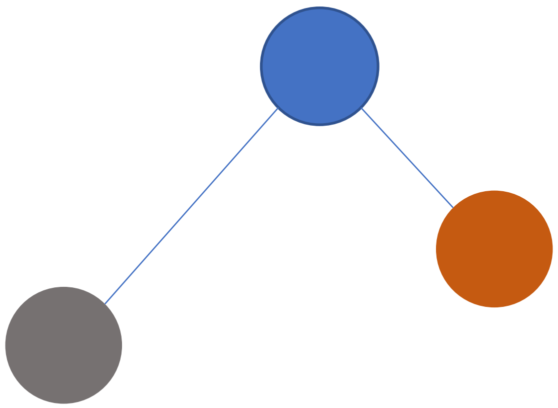


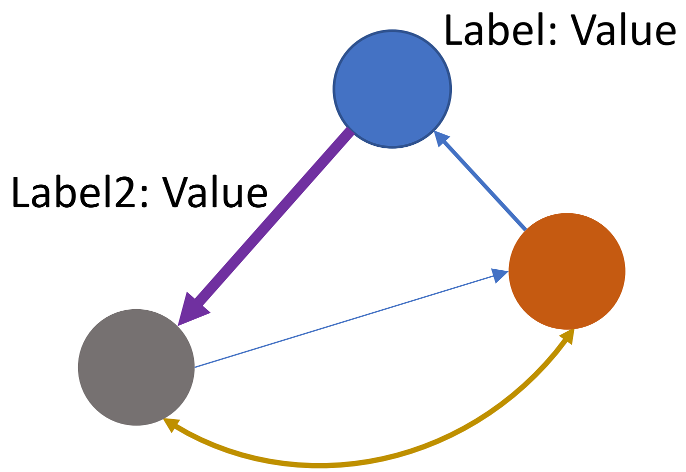
But…how do we learn from a graph?



Learning Frameworks and Graph Networks

- Manual approaches to feature engineering are complex and error prone
- Traditional ML frameworks do not scale efficiently to the size of the graph network when relationships are added





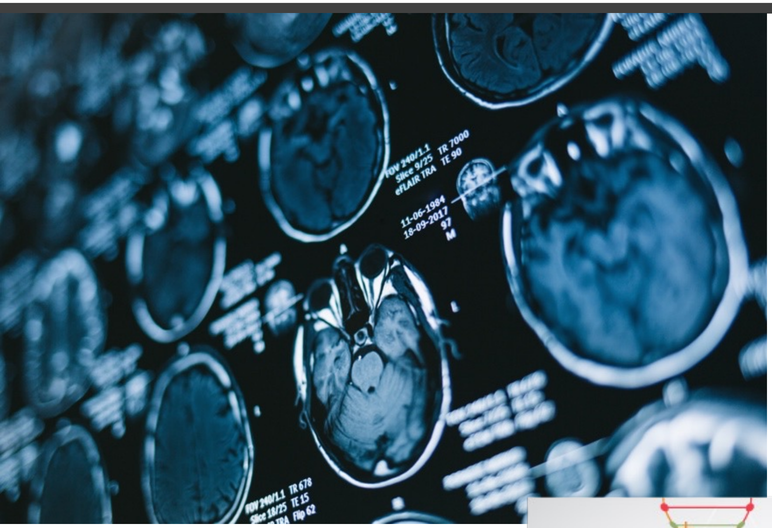
Stanford Graph Learning Workshop

Stanford ENGINEERING | Stanford Computer Forum

Stanford | Data Science

https://snap.stanford.edu/graphlearning-workshop/

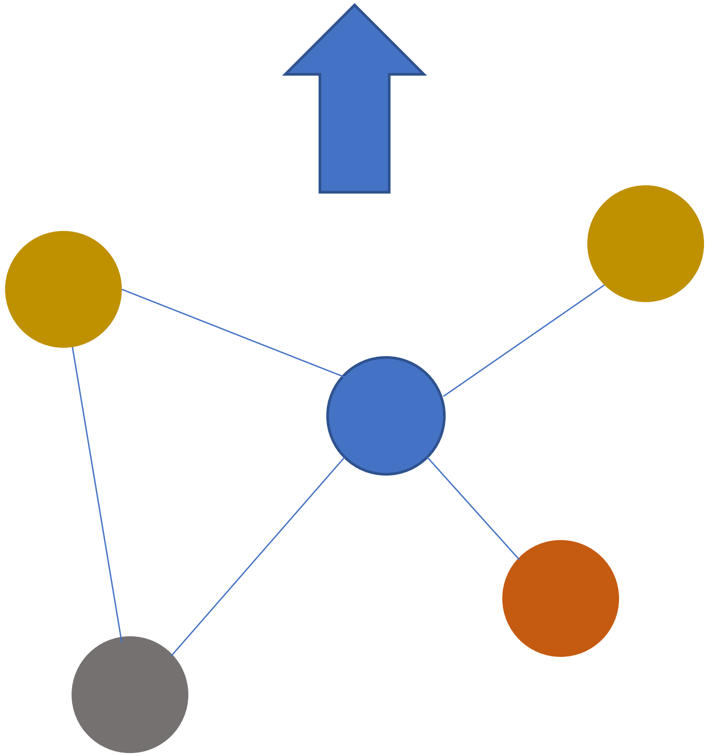
Applications of Graphs in Healthcare



Data to Knowledge to Insights

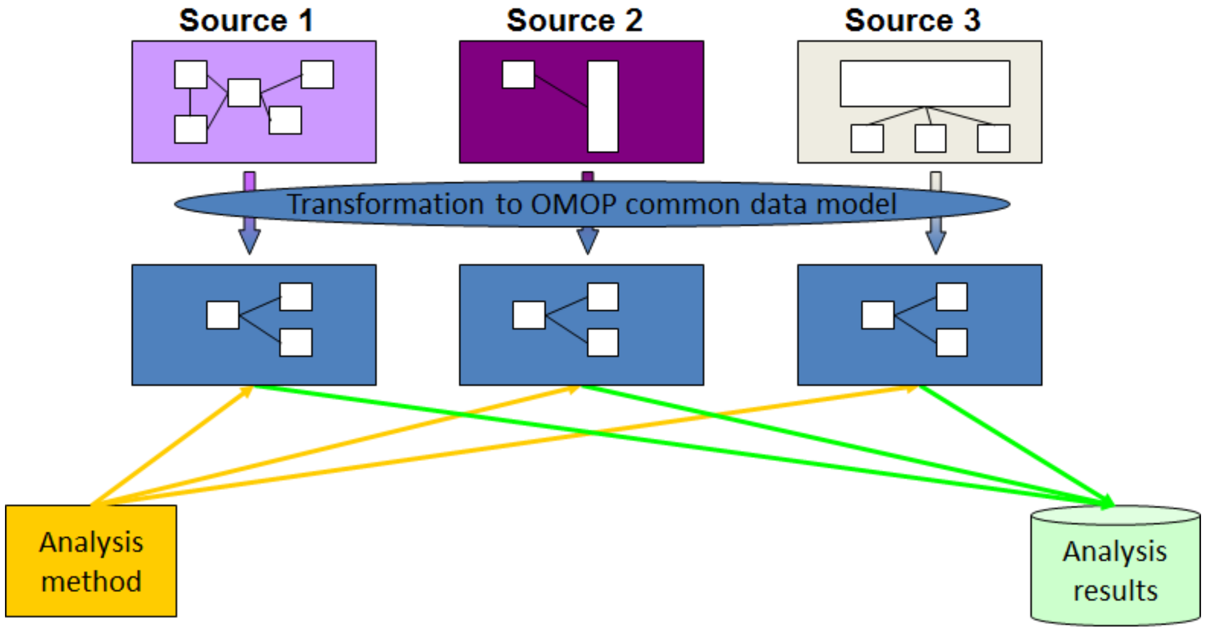
https://en.wikipedia.org/wiki/DIKW_pyramid#/media/File:DIKW_Pyramid.svg

Wisdom / Insight



Typical Healthcare Data Models

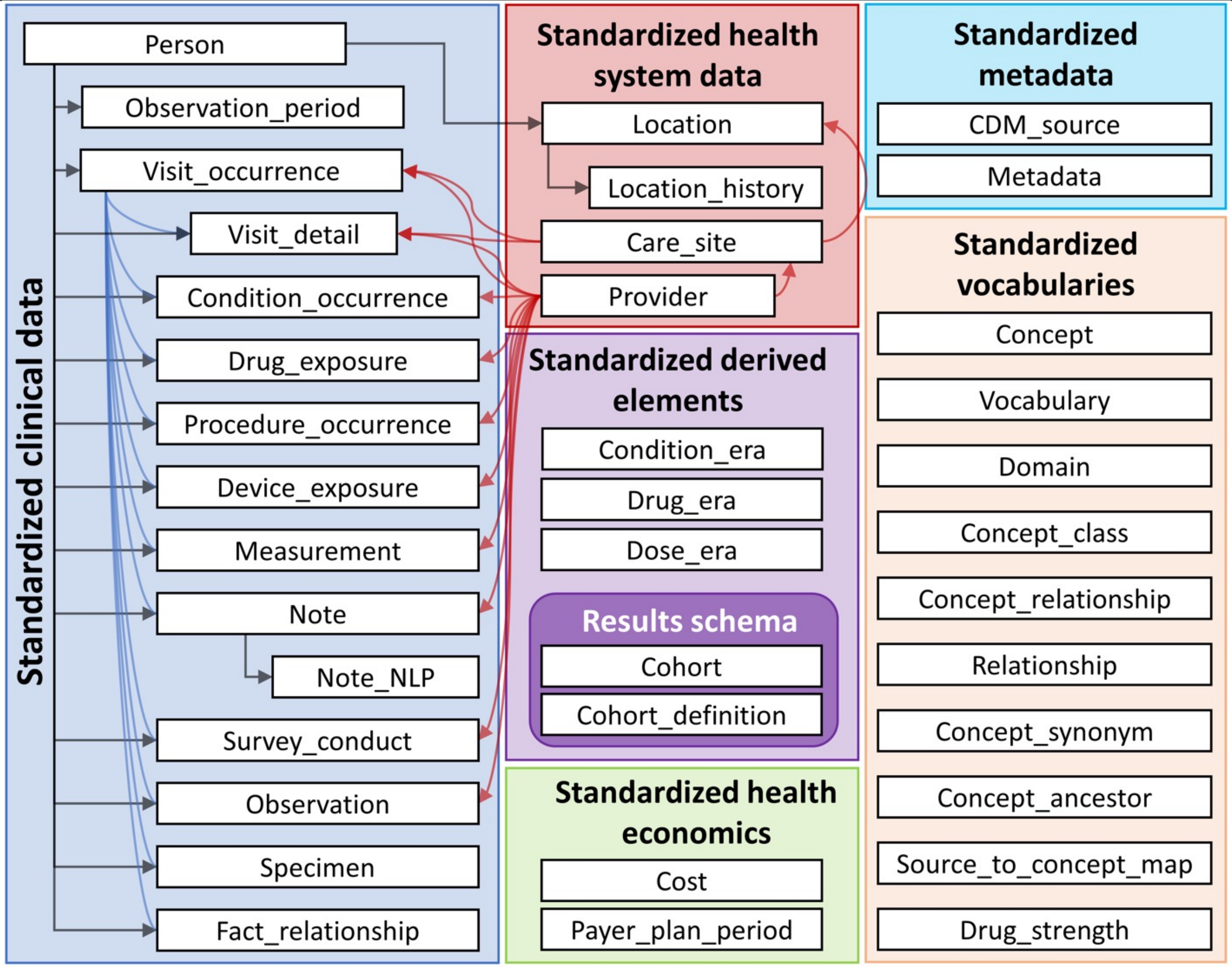
OBSERVATIONAL HEALTH DATA SCIENCES AND INFORMATICS



https://github.com/OHDSI

OHDSI and the OMOP Model

- Complex, relational data models
- Multiple dimensions and links, but little structure to automatically infer relationships and trajectory

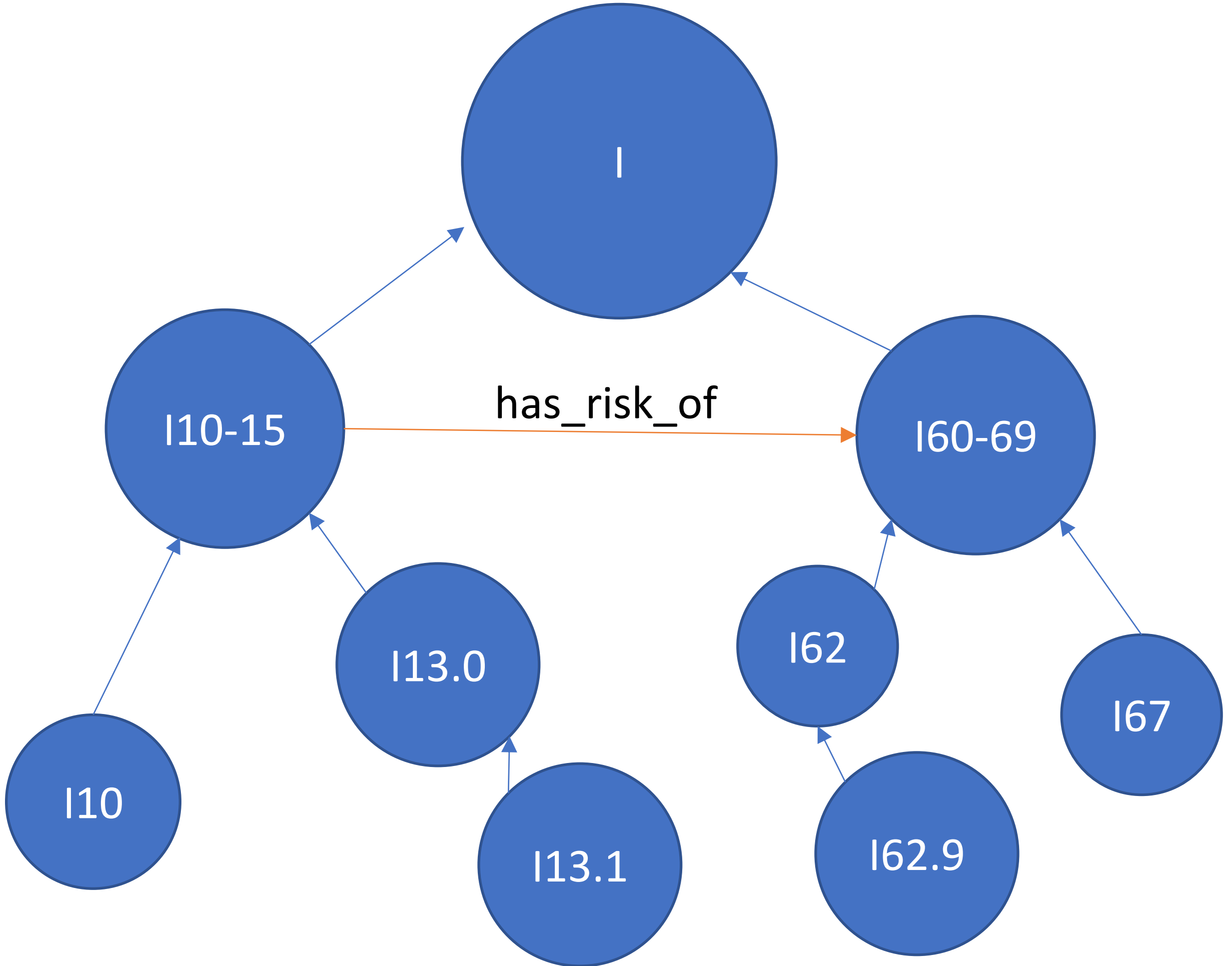


https://github.com/OHDSI/CommonDataModel
https://creatingrwe.thinkific.com/

Building Relationships for Health Data

Does patient 1 have a risk of stroke?

Patient ID	Diagnosis 1	Diagnosis 2
1	I13.1	
2	I62.9	I10
3	I10	I67

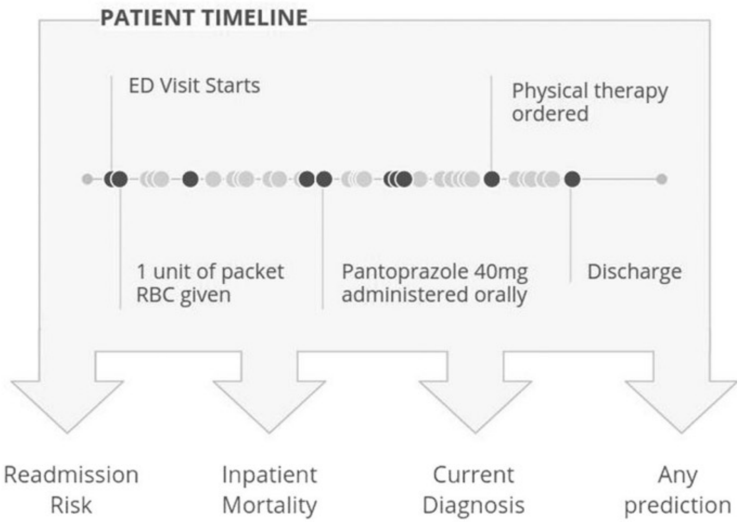


Advanced Models in Healthcare

Scalable and accurate deep learning with electronic health records

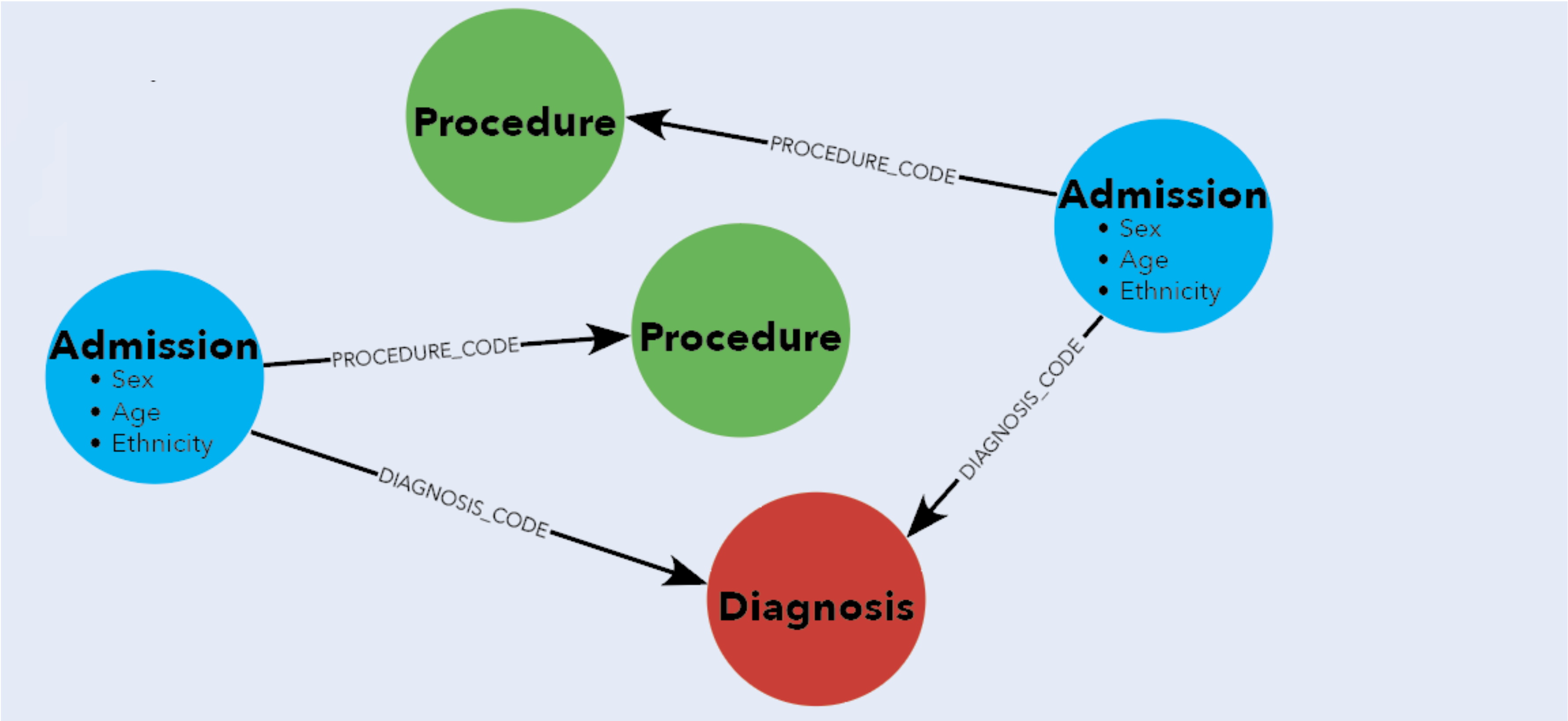
Alvin Rajkomar[1,2], Eyal Oren[1], Kai Chen[1], Andrew M. Dai[1], Nissan Hajaj[1], Michaela Hardt[1], Peter J. Liu[1], Xiaobing Liu[1], Jake Marcus[1], Mimi Sun[1], Patrik Sundberg[1], Hector Yee[1], Kun Zhang[1], Yi Zhang[1], Gerardo Flores[1], Gavin E. Duggan[1], Jamie Irvine[1], Quoc Le[1], Kurt Litsch[1], Alexander Mossin[1], Justin Tansuwan[1], De Wang[1], James Wexler[1], Jimbo Wilson[1], Dana Ludwig[2], Samuel L. Volchenboum[3], Katherine Chou[1], Michael Pearson[1], Srinivasan Madabushi[1], Nigam H. Shah[4], Atul J. Butte[2], Michael D. Howell[1], Claire Cui[1], Greg S. Corrado[1] and Jeffrey Dean[1]

https://www.nature.com/articles/s41746-018-0029-1.pdf



- Patient data from two hospitals in FHIR format, with each resource tokenized
- Each token is embedded, then concatenated for a single embedding per patient
- Trained three time-aware neural networks on four supervised tasks at three temporal points each

Easier with Graphs?



MIMIC in a Graph Model

Database | Credentialed Access

MIMIC-IV

Alistair Johnson, Lucas Bulgarelli, Tom Pollard, Steven Horng, Leo Anthony Celi, Roger Mark

Published: June 12, 2022. Version: 2.0

https://physionet.org/content/mimiciv/2.0/

- Semi-public data set
- Requires online/free privacy training and data use agreement
- Access to broad healthcare data from Beth Israel hospital in Boston, MA

MIMIC in a Graph Model

- Many graph database technologies, languages, and libraries to support graph modeling and AI applications
- For online code, using Neo4J and Python with data from MIMIC 3 (ICU data set) to predict length of stay

https://github.com/acomphealth/odsc2022-mimic-graphnet

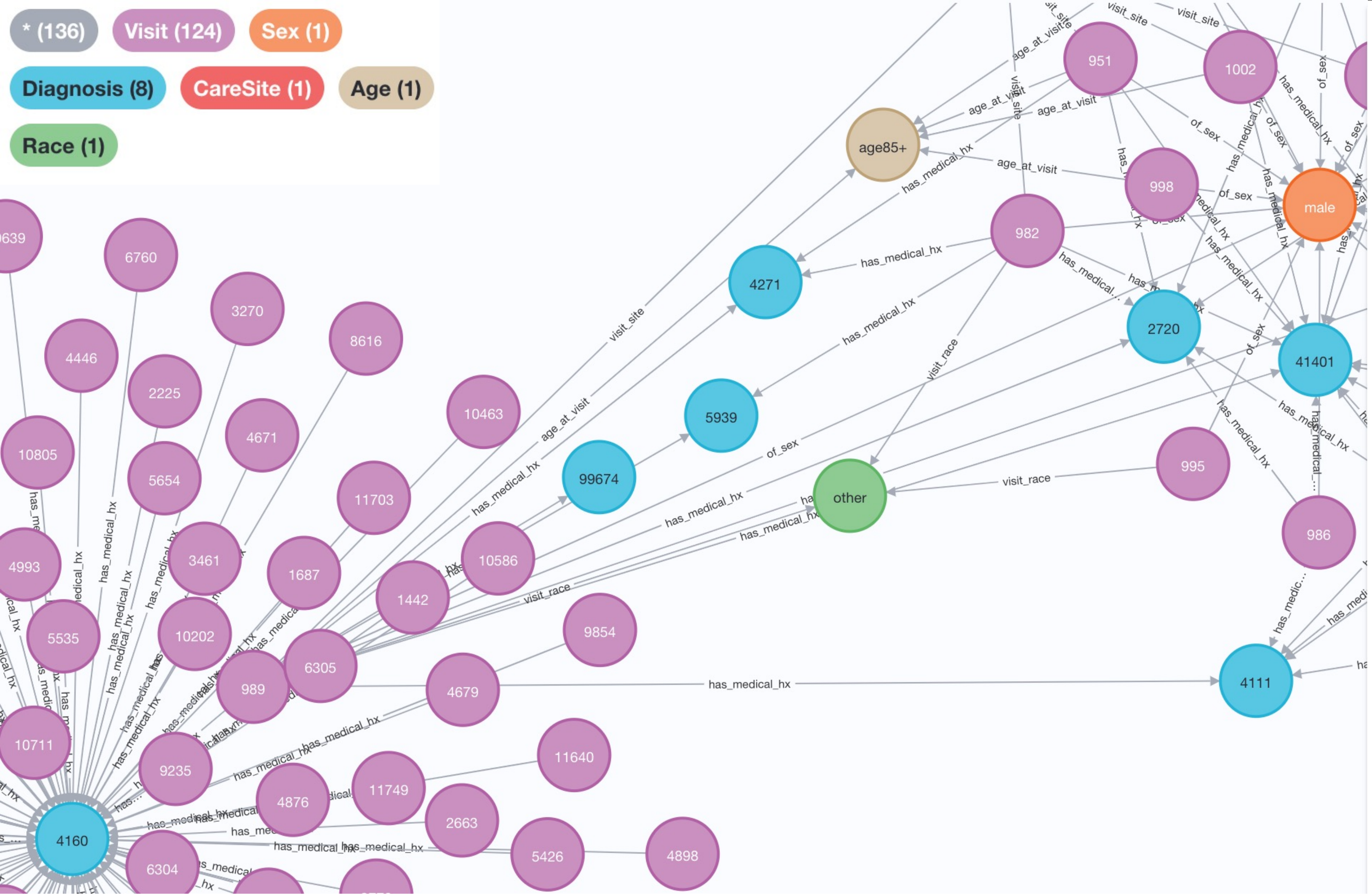
Modeling and Loading Data

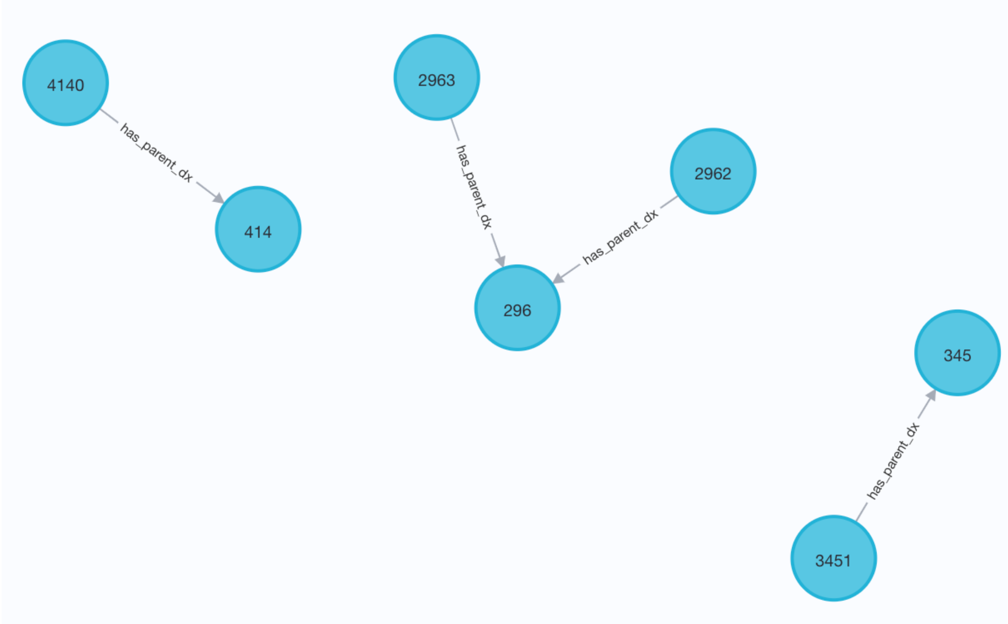
```
from neomodel import StructuredNode, StringProperty, ArrayProperty
from neomodel import RelationshipTo, RelationshipFrom


You, 1 second ago | 1 author (You)
class Visit(StructuredNode):
    visit_id = StringProperty(unique_index=True)
    embedding = ArrayProperty()

    sex = RelationshipTo("Sex", "of_sex")
    care_site = RelationshipTo("CareSite", "visit_site")
    race = RelationshipTo("Race", "visit_race")
    age = RelationshipTo("Age", "age_at_visit")

    dx = RelationshipTo("Diagnosis", "has_medical_hx")

You, 5 days ago | 1 author (You)
class Diagnosis(StructuredNode):
    icd = StringProperty(unique_index=True)
    embedding = ArrayProperty()

    child_dx = RelationshipFrom("Diagnosis", "has_parent_dx")
    parent_dx = RelationshipTo("Diagnosis", "has_parent_dx")
    visits = RelationshipFrom("Visit", "has_medical_hx")
```

- neomodel: Equivalent of relational database ORM – write model in code, map to graph

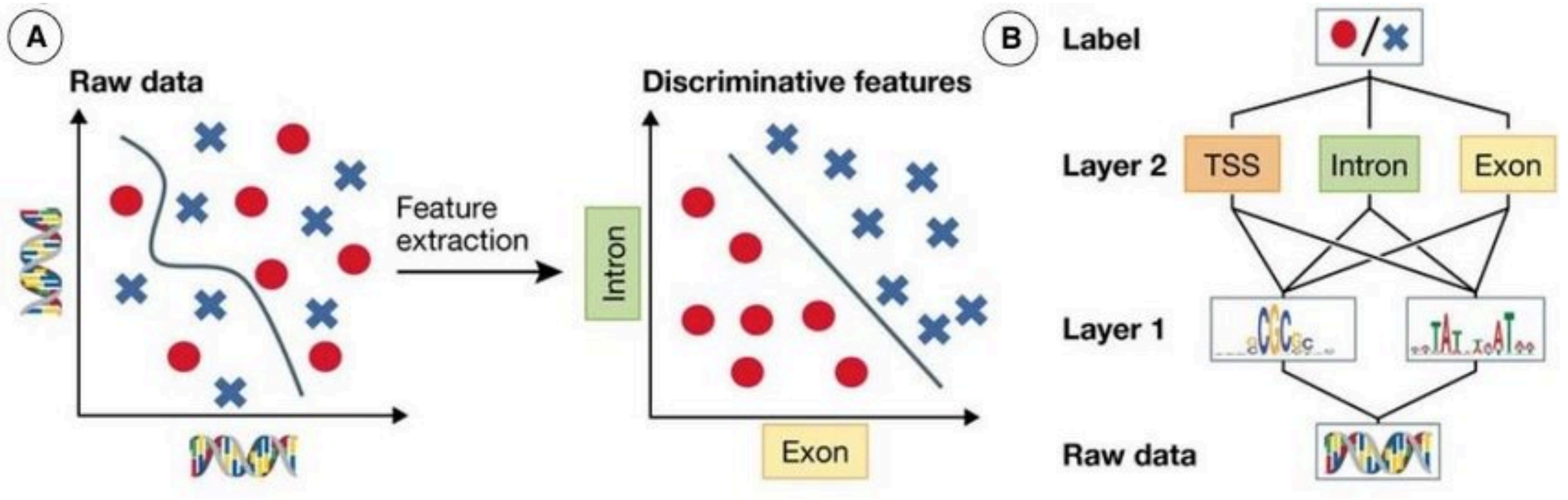
https://neomodel.readthedocs.io/en/latest/

Modeling and Loading Data





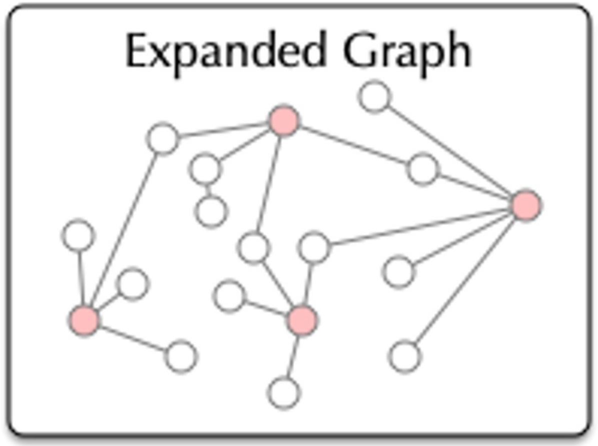
Efficiently Learning a Graph via Representation Learning

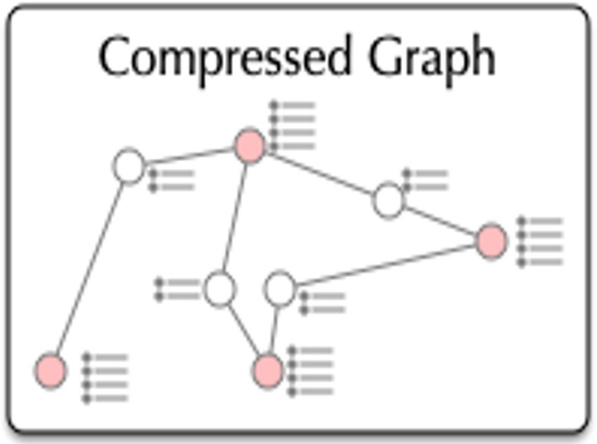


Kalinin et al: https://pubmed.ncbi.nlm.nih.gov/29697304/

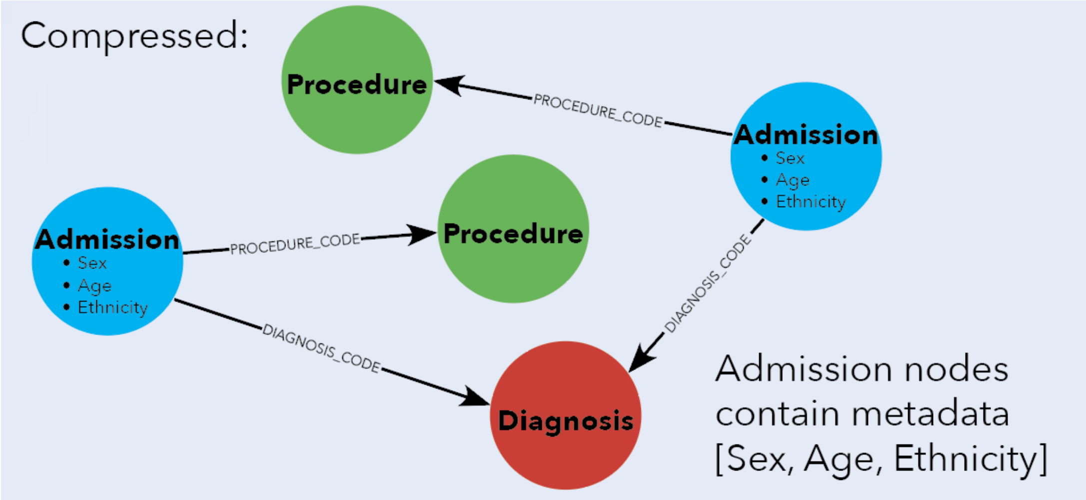
Question: Does our Graph Model Matter?

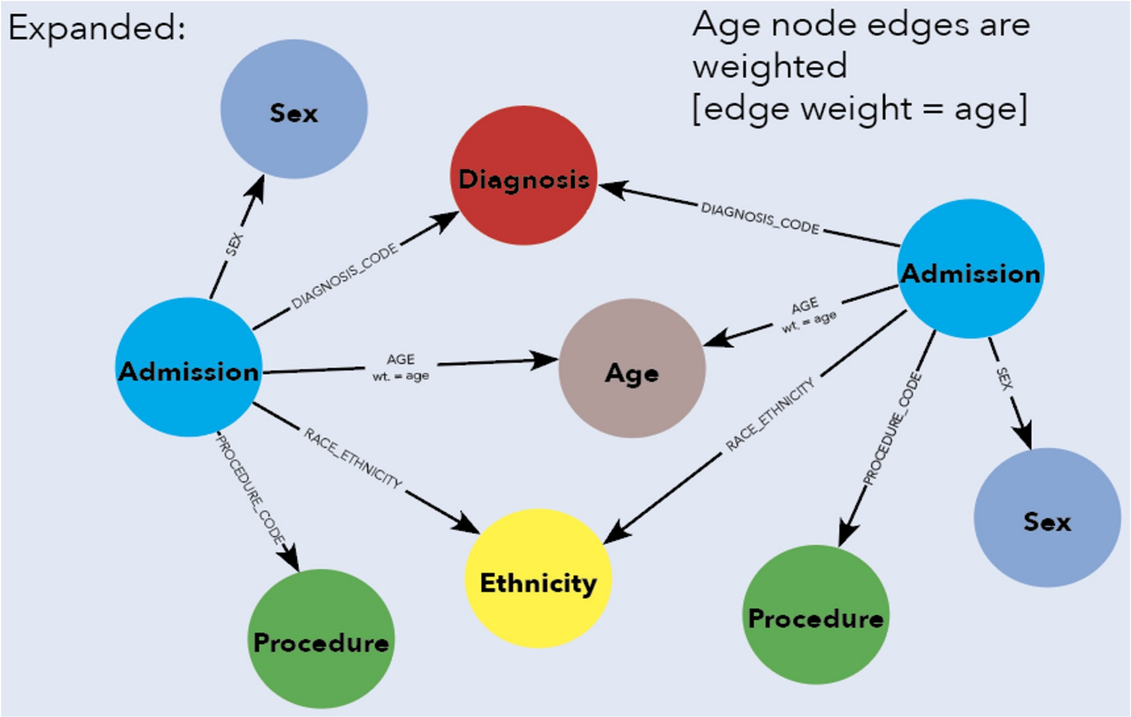
- One goal is to reduce the need for manual feature engineering
- But really, the goal is to shift some domain expertise effort from the data scientist to the data architect
- With representation learning and graph embeddings – choices in creating our data model might impact downstream predictive performance





Question: Does our Graph Model Matter?





Question: Does our Graph Model Matter?

- Inclusion Criteria:
  - Age on admission (90+ binned to 90)
  - Ethnicity/Race (top three (African American, Hispanic, White, binned Other)
  - Sex (Male/Female)
  - Diagnosis codes (top 100, summarized to the first 3 digits)
  - Procedure codes (top 40, summarized to the first 2 digits)
- Exclusion Criteria:
  - Age <18
  - Expired during visit

Question: Does our Graph Model Matter?

- Embeddings
  - Two embedding models implemented in Neo4J:
    - Node2Vec
    - GraphSAGE
  - Seven embedding sizes:
    - [20, 50, 100, 150, 200, 250, 300]
  - Two graph directions:
    - Directed, Undirected

- Predictive Model (80/20 train/test split)
  - Two predictive model architectures:
    - Random Forest
    - Logistic Regression
  - Outcome:
    - Length of Stay (<6 days/>6 days)

Using Neo4J GraphDataScience

```
print("Creating projected graph")
G, _ = gds.graph.project(
    'mimic',
    ['Visit', 'Sex', 'Race', 'Diagnosis', 'CareSite', 'Age'],
    ['age_at_visit', 'has_medical_hx', 'has_parent_dx', 'of_sex', 'visit_race', 'visit_site'],
    nodeProperties=["degree"]
)

print("Training GraphSAGE")
model, _ = gds.beta.graphSage.train(
    G,
    modelName = "mimicModel",
    learningRate = lr,       You, 3 days ago • refactor …
    epochs = 100,
    featureProperties = ["degree"]
)

print(model.metrics())

gds.beta.graphSage.write(
    G,
    writeProperty='embedding',
    modelName='mimicModel'
)
```

https://neo4j.com/docs/graph-data-science/current/

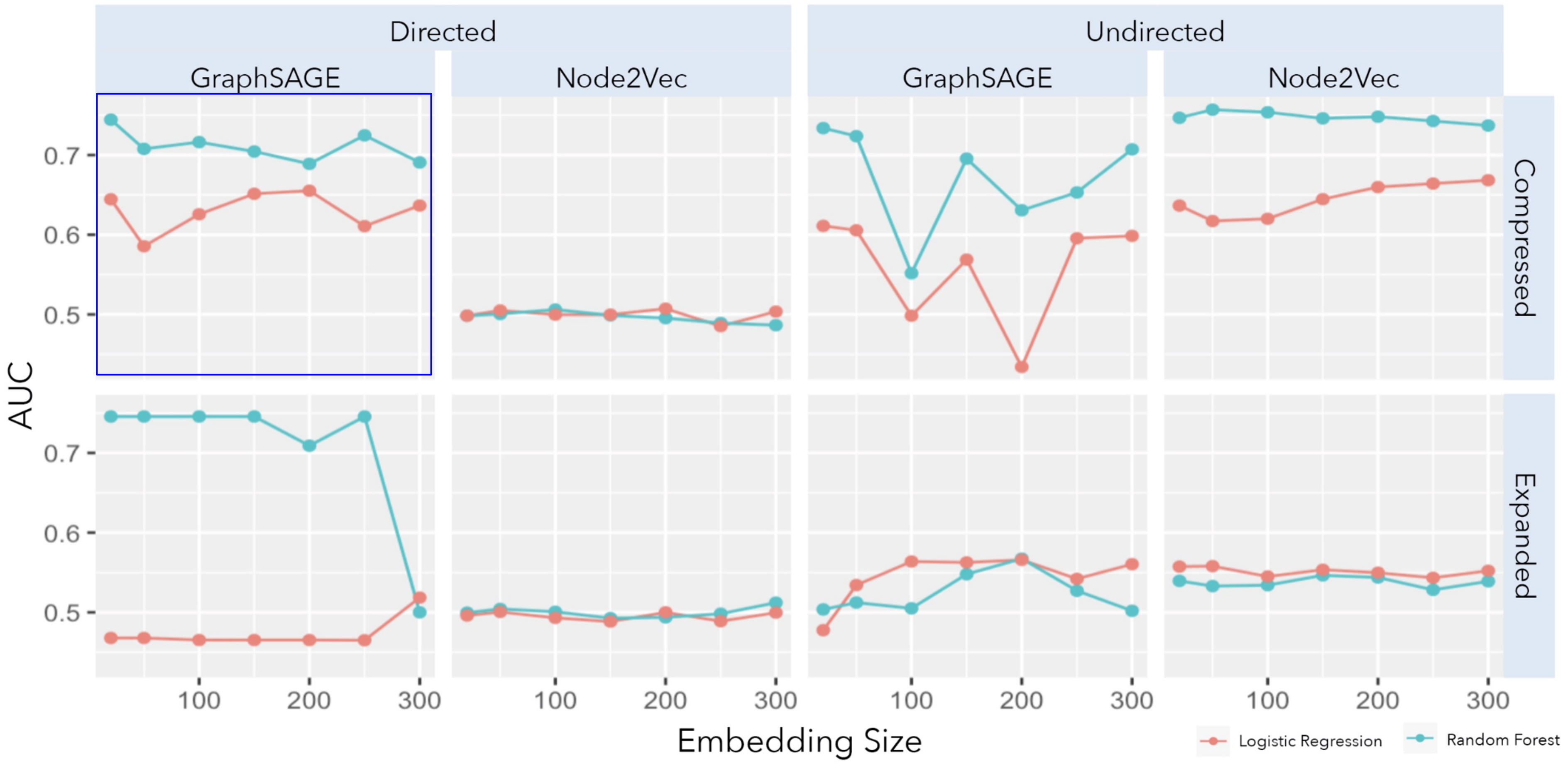
https://github.com/acomphealth/odsc2022-mimic-graphnet

MIMIC LOS Population Summary

n (%)

	LOS <6 days	LOS 6+ days	Overall
n	17,959	25,999	43,958
Sex M	10212 (56.9)	14639 (56.3)	24851 (56.5)
Age			
18-39	2538 (14.1)	2163 (8.3)	4701 (10.7)
40-51	2842 (15.8)	3470 (13.3)	6312 (14.4)
52-65	4960 (27.6)	7192 (27.7)	12152 (27.6)
66-76	3522 (19.6)	6355 (24.4)	9877 (22.5)
77-84	2404 (13.4)	4391 (16.9)	6795 (15.5)
85+	1693 (9.4)	2428 (9.3)	4121 (9.4)
Race & Ethnicity			
African American	1756 (9.8)	2284 (8.8)	4040 (9.2)
Hispanic	724 (4.0)	868 (3.3)	1592 (3.6)
Other	2885 (16.1)	4188 (16.1)	7073 (16.1)
White	12594 (70.1)	18659 (71.8)	31253 (71.1)

Graph Model and Prediction Accuracy



Graph Model Summary

- GraphSAGE > Node2Vec
  - Overall trend on either graph type or direction
  - Some approaches performed poorly, e.g., Node2Vec on directed graphs (possibly because it hinders the random walk)
- Compressed > Expanded
  - May be due to the age node being a central node that every visit connects to
  - Plan to explore use of binned ages
- Embedding size - minimal to no impact
- Random Forest vs Logistic Regression
  - RF better: 48%
  - LR better: 12.5%
  - Equivalent: 39.5%

Next Steps

- Convert age nodes to categorical buckets in expanded model (instead of one node with edge weights)
- Use knowledge graphs
  - Adding connections between all ICD code options (Procedure, Diagnosis)
    - from UMLS or OMOP concept hierarchies
    - ICD codes have notion of ordered diagnosis -> current graph with unconnected ICD codes cannot determine relationships
  - Primary diagnosis not currently separated out or weighted from secondary diagnoses

Communicating Graph Results

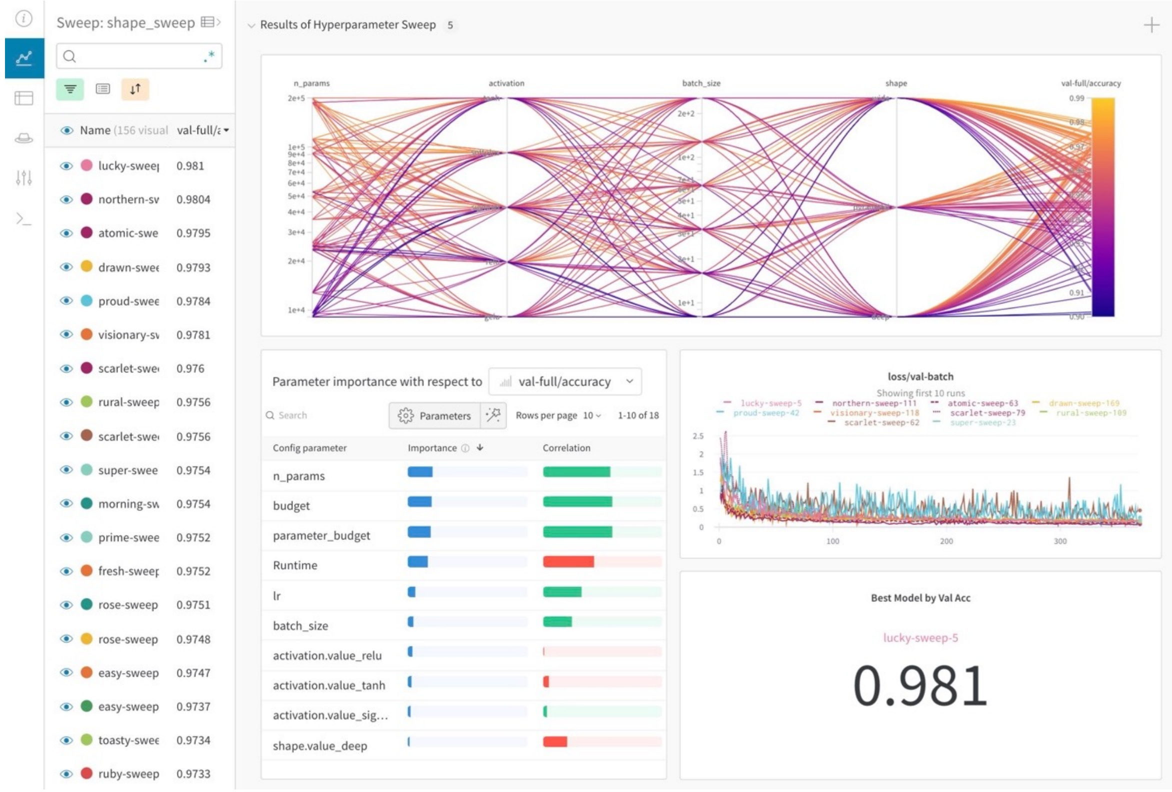
- Graph modeling can present additional challenges in communicating results compared to tabular data given the complexity of models and additional layers to the ML lifecycle
- Important to:
  - Document data sources
  - Describe population data, outcome frequency, and choices for both data modeling and predictive modeling parameters
  - Tooling exists to support logging of these data

Open-Source Tools for Graph AI

- PyTorch Geometric
  - Library built upon PyTorch to easily write and train Graph Neural Networks (GNNs) for a wide range of applications related to structured data
  - https://pytorch-geometric.readthedocs.io/en/latest/
- GraphGym
  - Platform for designing and evaluating GNNs
  - https://arxiv.org/pdf/2011.08843.pdf

https://pytorch-geometric.readthedocs.io/en/latest/notes/graphgym.html

Open-Source and Commercial MLOps



Conclusions

- Graph networks and graph AI is a rapidly growing field across academia and industry
- Graph models are complex and require new toolsets to efficiently train, evaluate, and use AI models
- Many industry use cases for graph networks, even within specialties in healthcare
- Important to tune not just hyperparameters, but also the data model when using graphs – these choices can impact downstream model performance
- Complexity of these models requires good documentation of data, parameter selection, and performance – visualizations help and tools exist to support this

Acknowledgements

- Sarah Dudgeon – PhD Student
- Katrin Hansel – Postdoctoral Associate
- Fred Warner – Associate Research Scientist
- Patrick Young – Associate Research Scientist
- Andreas Coppi – Associate Research Scientist
- Sameer Pandya – Data Scientist

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Questions?

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